Jastrow theory of the Mott transition in bosonic Hubbard models

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We show that the Mott transition occurring in bosonic Hubbard models can be successfully described by a simple variational wave function that contains all important long-wavelength correlations. Within this approach, a smooth metal-insulator transition is made possible by means of a long-range Jastrow correlation term that binds in real space density fluctuations. We find that the Mott transition has similar properties in two and three dimensions but differs in one dimension. We argue that our description of the Mott transition in terms of a binding-unbinding transition is of general validity and could also be applied to realistic electronic systems.

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Stimulated by the discovery of many strongly-correlated materials which, on the verge of becoming Mott insulators, display interesting and unusual properties, a huge theoretical effort has been devoted in the last decades to clarify the interaction-driven Mott metal-insulator transition (MIT). [1] In spite of that, a full comprehension of this phenomenon is still lacking, even though, in the limit of infinite-coordination lattices, the whole dynamical behavior across the MIT can be uncovered thanks to Dynamical Mean-Field Theory. [2] As a matter of fact, the Mott phenomenon is not specific of fermions but also occurs in bosonic systems, [3] that have recently become popular in the context of optical lattices, where a MIT can be actually realized experimentally. [4]

The prototypical Hamiltonian to describe a MIT both for fermions and bosons is the Hubbard model

$$\mathcal{H} = -\sum_{ij,\,\sigma}\left(t_{ij}\, b^{\dagger}_{i\sigma} b_{j\sigma} + H.c.\right) + \frac{U}{2}\sum_{i} n_i\,(n_i-1), \quad (1)$$

where $b^{\dagger}_{i\sigma}$ ($b_{i\sigma}$) creates (annihilates) a particle at site i with spin $\sigma = -S, \ldots, S$, being S half-odd-integer for fermions and integer for bosons and $n_i = \sum_\sigma b^{\dagger}_{i\sigma} b_{i\sigma}$ the local density operator. The Hubbard model (1) at commensurate densities generally shows two different phases: If $U < U_c$ particles are delocalized, which implies a metallic behavior for fermions (unless a Stoner instability leads to magnetically ordered phases) and superfluidity for bosons; instead, when $U > U_c$ the model describes a Mott insulator where coherent motion is suppressed. Presumably, for any $S \neq 0$, the Mott insulating phase is accompanied by translational and eventually spin-rotational symmetry breaking. However, the latter is merely a consequence of the Mott phenomenon and should not be identified as the driving mechanism leading to the insulating behavior, which arises from a strong suppression of charge fluctuations. Indeed, a MIT does occur also for $S = 0$ bosons, in which case no symmetry breaking is expected within the Mott insulator. In this work we focus on the bosonic Hubbard model by describing the Mott phase with a strongly correlated variational wave function. An advantage of considering bosons is that we can directly compare the variational outcome with numerically exact results obtained by Green's function Monte Carlo (GFMC). [5, 6] Therefore, by means of this comparison, we can establish the key ingredients that must be included in the variational state for a faithful representation of a genuine Mott insulating state.

In spite of the fact that the variational approach is a simple and well established technique, its application to the MIT turns out to be extremely difficult. For instance, the celebrated Gutzwiller wave function $|\Psi_G\rangle = \prod_i \gamma(n_i)|\Phi_0\rangle$, where $|\Phi_0\rangle$ is the non-interacting ground state and $\gamma(n_i)$ is an operator which progressively suppresses expensive occupancies, is not appropriate to describe the MIT in both fermionic and bosonic cases. [7, 8] Indeed, the only way to produce an insulating wave function corresponds to project out completely on-site occupancies different from the average one. This wave function, with no charge fluctuations, is clearly a very poor description of a realistic Mott insulator. In fact, for the fermionic Hubbard model, the optimal $|\Psi_G\rangle$ is never insulating, except at $U = \infty$, even if the variational wave function is improved by adding short-range density-density correlations. [7, 9] In the case of $S = 0$ bosons, an insulating $|\Psi_G\rangle$ can be stabilized at finite U, [8] but, as we mentioned, the insulator obtained in this way gives an incorrect description of the actual ground state.

A step forward has been recently accomplished in one dimension, where it has been shown [10] that a Gutzwiller wave function supplemented by a *long-range* Jastrow factor offers a very accurate description of a Mott insulator. However, a systematic analysis of this variational ansatz in higher dimensions is still lacking, while it would be highly desirable in view of more realistic applications. In this letter, we apply this variational approach to the $S = 0$ bosonic Hubbard model (1) with nearest-neighbor hopping $t/2$ in a one-dimensional chain (1D), a two-dimensional (2D) square lattice and a three-dimensional

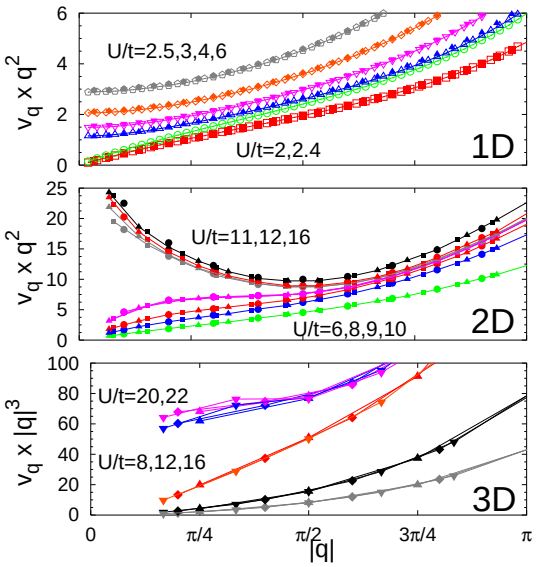

FIG. 1: Variational results for the Jastrow potential v_q multiplied by q^2 in 1D and 2D and by $|q|^3$ in 3D for increasing values of U/t (from bottom to top). Upper panel: 1D case for 60 and 100 sites. Middle panel: 2D case for 20×20, 26×26, and 30×30 clusters (along the $(1,0)$ direction). Lower panel: 3D case for $8\times 8\times 8$, $10\times 10\times 10$, and $12\times 12\times 12$ clusters (along the $(1,0,0)$ direction).

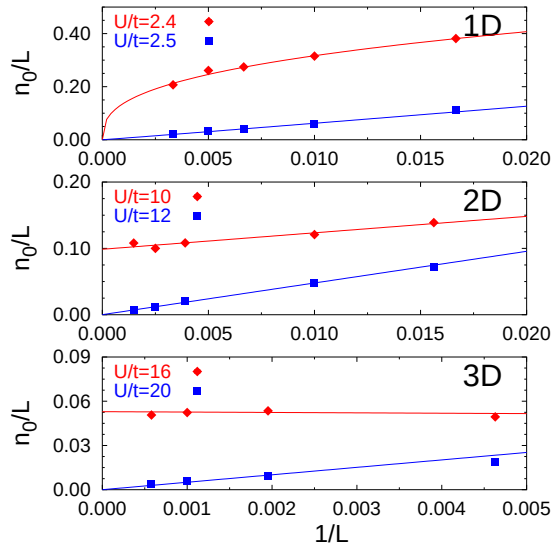

FIG. 2: Variational values of the condensate fraction $\mathtt{n}_0/L$ in 1D (upper panel), 2D (middle panel), and 3D (lower panel).

(3D) cubic lattice with L sites. Specifically, we consider the following ansatz for the variational wave function

$$|\Psi\rangle = \exp\left(-\frac{1}{2}\sum_{i,j} v_{i,j} n_i n_j + g_{MB}\sum_i \xi_i\right)|\Phi_0\rangle, \quad (2)$$

where $|\Phi_0\rangle$ is the non-interacting fully-condensed wave function, i.e. $|\Phi_0\rangle = (b^\dagger_{k=0})^N|0\rangle$, being $b^\dagger_k$ the creation operator at momentum k and N the number of particles. In the following, we will consider $N = L$. The components of the Jastrow potential, $v_{i,j} = v(|R_i - R_j|)$, are independently optimized by minimizing the variational energy, [11] and we will denote by n_q and v_q the Fourier transforms of the local density n_i and of $v_{i,j}$, respectively. Finally, g_{MB} is a variational parameter related to the many-body operator $\xi_i = h_i\prod_\delta(1-d_{i+\delta}) + d_i\prod_\delta(1-h_{i+\delta})$, where $h_i = 1$ ($d_i = 1$) if the site i is empty (doubly occupied) and 0 otherwise, and δ is the vector which connects nearest-neighbor sites; [12] in other words, $\sum_i \xi_i$ counts the number of isolated empty and doubly occupied sites. This term is kept mainly to improve the variational accuracy (in 2D and 3D) but does not introduce important correlation effects, that are instead contained only in the *long-range* behavior of the two-body Jastrow potential $v_{i,j}$. Remarkably, it turns out that our wave function (2) is quite accurate in all cases that we considered, even across the MIT; more details will be reported elsewhere. [13]

Let us start by discussing the relevance of the Jastrow factor for the low-energy properties and some expected asymptotic behaviors of v_q. In the gapless (superfluid) phase, a long-range Jastrow potential is surely needed to restore the correct small-q behavior of the static density structure factor, i.e., $N_q = \langle\Psi|n_{-q}n_q|\Psi\rangle/\langle\Psi|\Psi\rangle \sim |q|$. Indeed, since at least in the weak-coupling regime, the expression

$$N_q = \frac{N_q^0}{1+\gamma\, v_q\, N_q^0} \quad (3)$$

holds with $\gamma = 2$, [14] where the non-interacting $N_q^0 = \langle\Phi_0|n_{-q}n_q|\Phi_0\rangle/\langle\Phi_0|\Phi_0\rangle \sim$ const, it follows that $v_q \sim 1/|q|$. The same asymptotic behavior was obtained in Refs. [10, 15, 16] by full optimization of v_q in metallic fermionic models both in 1D and 2D, where both $N_q \sim |q|$ and $N_q^0 \sim |q|$. Moreover, it was shown that, in the insulating phase, a more singular $v_q \sim 1/q^2$ at small q is required to recover the appropriate $N_q \sim q^2$ insulating behavior, consequence of exponentially decaying correlation functions. This similarity between 1D and 2D fermionic models was suggestive that $v_q \sim 1/q^2$ is sufficient to induce an insulating behavior in any dimensions as well as that the expression (3) remains asymptotically valid for $|q| \to 0$, even inside the insulating regime at strong coupling. However, one easily realizes that, were this conclusion correct, the variational wave function (2) could not describe any bosonic insulator in 3D, since $v_q \sim 1/q^2$ is not sufficient to empty the condensate fraction $\mathtt{n}_0 = \langle\Psi|b^\dagger_{k=0}\, b_{k=0}|\Psi\rangle/\langle\Psi|\Psi\rangle$. [17] Instead, we will show that our Jastrow wave function can give a consistent description of the Mott phase *in any dimension* thanks to an even more diverging v_q, implying that

the formula (3) can be violated in the real 3D world.

In Fig. 1 we present the optimized Jastrow potential v_q. For all dimensions, the MIT can be clearly detected from the sudden change in the small-q behavior of v_q. On the one hand, the gapless superfluid phase is always described by $v_q \sim \alpha/|q|$, with α increasing with U. On the other hand, the gapped insulator has a much more diverging v_q. In 1D we recover the $v_q \sim 1/q^2$ behavior, like in the fermionic case. [10] In 2D, the leading behavior of the Jastrow potential across the transition is less clearcut than in 1D. Indeed, we cannot establish whether, on the insulating side, $v_q \sim \beta_{2D}/q^2$ with β_{2D} large but finite, or possible logarithmic corrections have to be considered, i.e., $v_q \sim \ln(1/|q|)/q^2$. The first possibility is particularly appealing since, in this case, the insulating phase can be interpreted in terms of the confined phase of the 2D classical Coulomb gas. [16, 18] Notice that the optimized v_q, that also contains subleading corrections to the $1/q^2$ behavior, can modify the critical properties of the classical Coulomb gas model. Nevertheless, the essential point is that, within this approach, the MIT can be still interpreted in terms of a binding-unbinding transition among charged particles (empty and doubly occupied sites). Finally, in 3D an even more diverging v_q is stabilized in the insulating regime, i.e., $v_q \sim 1/|q|^3$. Therefore, in all these cases the Jastrow potential is sufficient to destroy the condensate (see Fig. 2). [19]

In order to verify the validity of our approach, let us move to discuss the variational results for the density structure factor N_q in comparison with the exact ones obtained by GFMC. For small q's we can generally write $N_q = \gamma_1|q| + \gamma_2 q^2 + \mathrm{O}(q^3)$. In analogy with spin systems, we may assume that $\gamma_1 = v_c\,\chi$, being v_c and χ the charge velocity and the compressibility, respectively. At the variational level γ_1 and γ_2 depend crucially upon the Jastrow parameters. Indeed, we do find that, in the superfluid phase, $\gamma_1 \neq 0$ while, in the Mott insulator, $\gamma_1 = 0$ and $\gamma_2 \neq 0$, signaling that this state is incompressible (see Fig. 3). Moreover, in 1D we have evidence for a jump (from a finite value to zero) in γ_1 across the MIT, especially because its value does not change much passing from $U = U_c/2$ and $U \lesssim U_c$ (e.g., it changes from 0.4 to 0.2). These variational results are confirmed by GFMC and are consistent with the finite jump of the compressibility across the Kosterlitz-Thouless transition, expected in 1D. [3] Our numerical results seem also to indicate that γ_2 diverges as the MIT is approached from the insulating side. In the variational calculation, this behavior follows from a $v_q \sim \beta_{1D}/q^2$ in the insulating phase with $\beta_{1D} \to 0$ at the MIT. In conclusion we find that the 1D MIT can be located at $U_c/t \simeq 2.45$ in the variational calculations, whereas the GFMC gives $U_c/t \simeq 2.2$ (in close agreement with previous calculations of Ref. [20, 21]), showing that the variational wave function (2) is not only qualitatively but also quantitatively correct.

The density structure factor N_q displays quite distinct

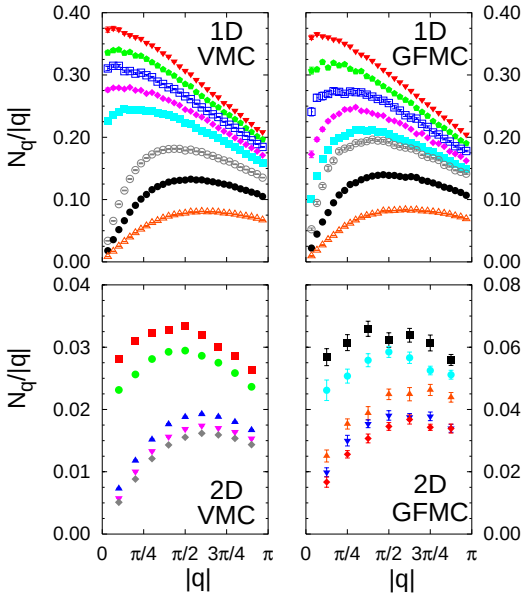

FIG. 3: Density structure factor N_q divided by $|q|$ calculated with variational Monte Carlo (left panels) and GFMC (right panels) in 1D (upper panels) and 2D (lower panels) In 1D, $L = 60$ and $U/t = 1.6$, 1.8, 2, 2.2, 2.4, 2.5, 3, and 4. In 2D, $L = 20 \times 20$ and $U/t = 10$, 10.2, 10.4, 10.6, and 10.8 for the variational calculation, and $L = 256$ and $U/t = 8$, 8.2, 8.4, 8.6, and 8.8 in the GFMC calculation. All cases are shown from top to bottom for increasing values of U/t.

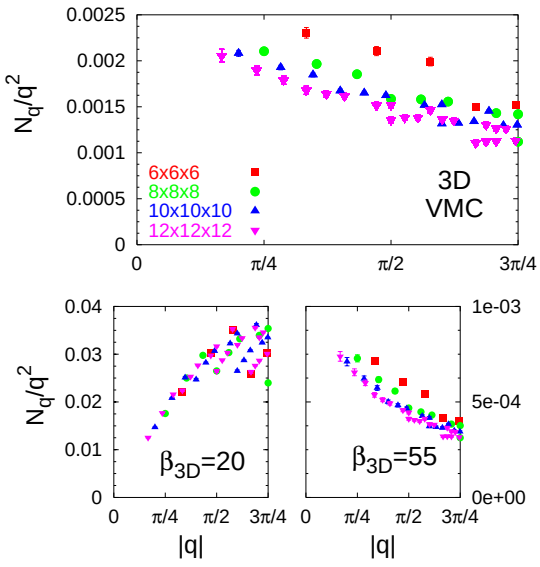

FIG. 4: Upper panel: Density structure factor N_q divided by q^2 calculated by the variational Monte Carlo for 3D and $U/t = 20$. Lower panels: N_q for non-optimized wave functions with $v_q \sim \beta_{3D}/|q|^3$ for two values of β_{3D} and the same sizes as above.

long-wavelength behaviors for weak and strong interactions also in 2D, see Fig. 3. In the variational calculations, for $U/t \lesssim 10.3$ the structure factor goes like $N_q \sim \gamma_1 |q|$, while for $U/t \gtrsim 10.3$ we get $N_q \sim \gamma_2 q^2$. The critical value of the on-site interaction is slightly different from the GFMC one, which we find to be $U_c/t \simeq 8.5$, in agreement with Ref. [22]. In spite of the different values of U_c, the qualitative behavior across the MIT is similar both in the variational and in the GFMC calculations. It should be emphasized that in 2D the value of γ_1 close to the MIT is one order of magnitude smaller than its value at $U/U_c \sim 1/2$, a behavior qualitatively different from 1D, suggesting that γ_1 vanishes upon approaching the MIT from the superfluid side and that γ_2 is smooth and constant across the MIT in 2D.

More interesting is the 3D case. Here, the GFMC is severely limited by small sizes and, therefore, we will just discuss the variational results. The change in the leading behavior of the Jastrow parameters v_q allows us to locate the transition around $U_c/t \simeq 18$, which is very close to the critical value extracted from experiments on optical lattices. [4] The optimal Jastrow potential behaves as usual as $v_q \sim \alpha/|q|$ in the superfluid phase, but turns into $v_q \sim \beta_{3D}/|q|^3$ in the Mott insulator (see Fig. 1). This behavior would imply, if Eq. (3) were valid, a charge structure factor $N_q \sim |q|^3$. By contrast, we do find that $N_q \sim q^2$, as expected in an insulator, see Fig. 4. So, we arrive at the very surprising and unexpected result that Eq. (3) does not hold, not even asymptotically for $|q| \to 0$. In order to prove more firmly that a $v_q \sim \beta_{3D}/|q|^3$ can indeed lead to $N_q \sim q^2$, we have calculated N_q with a non-optimized wave function of the form (2) with $v_q \sim \beta_{3D}/|q|^3$, for different values of β_{3D}. As shown in Fig. 4, for small β_{3D}'s $N_q \sim |q|^3$, implying that Eq. (3) is qualitatively correct. However, above a critical β^*_{3D}, the behavior turns into $N_q \sim q^2$, signaling a remarkable breakdown of Eq. (3). The optimal value of β_{3D} that we get variationally at the MIT is larger than β^*_{3D}, confirming our variational finding $N_q \sim q^2$. We notice that the change of behavior as a function of β_{3D} is consistent with the binding-unbinding phase transition recently uncovered in a classical 3D gas with potential $V_{\rm cl}(q) \sim 1/|q|^3$. [23]

In conclusion we have demonstrated that a long-range Jastrow potential does allow for a faithful variational description of a Mott transition in the bosonic Hubbard model, in spite of the fact that the uncorrelated wave function onto which the Jastrow factor is applied has full Bose-condensation. An interesting outcome of our analysis is that, in 3D, the Mott insulator is characterized by a very singular Jastrow potential, $v_q \sim 1/|q|^3$, that is able to empty the condensate, yet leading to a well behaved charge structure factor, $N_q \sim q^2$. This result contradicts the naïve expectation, $N_q \sim 1/v_q$, based on the weak-coupling formula (3). This breakdown of the weak-coupling approach is the necessary condition for our wave function to work in 3D and represents a highly nontrivial consistency check of our non-perturbative variational theory of the Mott phase. We argue that this variational theory will hold also in electronic models. In particular, once the square of the ground state wave function is interpreted as a classical partition function, the metal-insulator transition can be induced in any dimension by a singular interaction between charge fluctuations. Remarkably, in $D > 1$ this interaction remains always logarithmic, suggesting an unconventional binding-unbinding description of the metal-insulator transition. In analogy with the bosonic example we have analyzed, we should expect that a singular Jastrow potential, $v_q \sim 1/|q|^\theta$ with $\theta = 3$, might be necessary to describe the 3D Mott transition in fermionic models, too, all the more reason when realistic Coulomb interaction is taken into account.

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